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ION PAIR SOLVATION

FINAL REPORT

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New tools for the computational simulation of ion and ion-pair dynamics in the gas phase and in solution have been developed. Both classical and quantum mechanical methods were explored. Monte-Carlo techniques for incorporating thermodynamic equilibrium effects of surrounding solvent molecules have been incorporated into the computer codes. New techniques for computing highly accurate weak interaction energies among anions and solvent molecules have been developed and tested.

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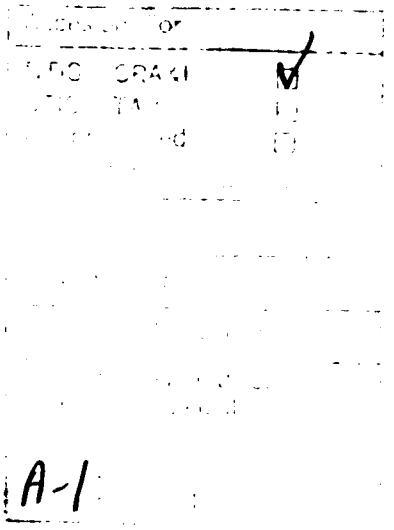
The general problem on which our efforts were focused during this grant period dealt with the solvation of ions and ion pairs. We explored the fundamental intermolecular interaction energies among the ion (or ions) and the surrounding solvent molecules. Statistical methods for incorporating the effects of thermodynamic fluctuations in the solvent molecules were also built into our computer simulation capabilities. Finally classical and quantum dynamics tools were used to simulate and study the time evolution of solvent clustered ion pairs which have been excited either thermally or by photochemical means.

The primary result of findings of this grant are detailed in the publications listed below. The names of the people who worked on these projects are also given below. The primary achievement of this effort is the development of state-of-the-art computer simulation techniques for the study of structural, energetic, thermodynamic, and dynamic properties of ions and ion pairs in solution. Earlier progress reports, including the final progress report submitted in August of 1988 provide further details on the specific ions and on pairs which we studied.



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LIST OF MANUSCRIPTS SUBMITTED OR PUBLISHED UNDER ARO SPONSORSHIP DURING THIS REPORTING PERIOD, INCLUDING JOURNAL REFERENCES:

"Rotational Predissociation of Model Atom-Diatom Complexes," R. F. Frey, J. O. Jensen and J. Simons, J. Phys. Chem. 89, 788 (1985).

"Translational and Rotational Symmetries in Integral Derivatives of Arbitrary Order,", J. O. Jensen, A. Banerjee and J. Simons, Chem. Phys. 102, 45-54 (1986).

A Different View of Molecular Electronic Transitions," H. Taylor and J. Simons, J. Phys. Chem. 90, 580.

"Resonance state energies and lifetimes via analytic continuation of stabilization graphs," R. F. Frey and J. Simons, J. Chem. Phys. 84, 4462 (1986).

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"Fragmentation Dynamics of Solvent-Clustered Ion Pairs," R. F. Frey and J. Simons, J. Phys. Chem. 91, 2818 (1987).

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"Ab initio studies of the structures and energies of the $H^-(H_2O)$ and $H^-(H_2O)_2$ complexes," G. Chalasinski, R. A. Kendall and J. Simons, J. Chem. Phys. 87, 2965 (1987).

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"A unitary multiconfigurational coupled-cluster method: Theory and applications," Mark R. Hoffmann and Jack Simons, J. Chem. Phys. 88, 993 (1988).

SCIENTIFIC PERSONNEL SUPPORTED BY THIS PROJECT AND DEGREES AWARDED DURING THIS REPORTING PERIOD:

Grzegorz Chalasinski
Mark Hoffmann
Rick A. Kendall
Doug O'Neal
Hugh Taylor
Ramon Hernandez
Edward Earl

No advanced degrees were awarded during this reporting period.